

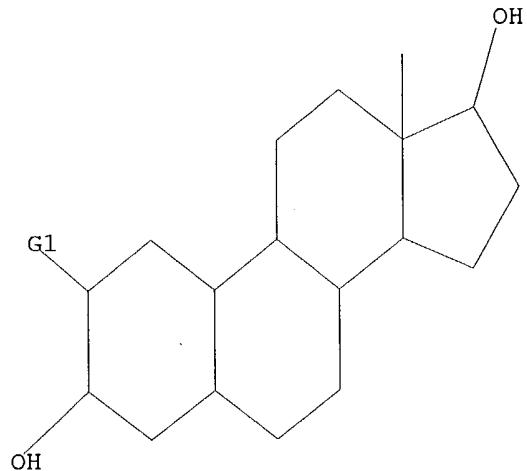
chain nodes :
18 19 20 21
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
chain bonds :
2-21 3-20 13-18 15-19
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10
11-12 12-13 13-14 13-15 14-17 15-16 16-17
exact/norm bonds :
2-21 3-20 15-19
exact bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10
11-12 12-13 13-14 13-15 13-18 14-17 15-16 16-17
isolated ring systems :
containing 1 :

G1:X,Ak,S,N,MeO,EtO,n-PrO,i-PrO

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:CLASS 19:CLASS 20:CLASS 21:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 X, Ak, S, N, MeO, EtO, n-PrO, i-PrO

Structure attributes must be viewed using STN Express query preparation.

```
=> s 11
SAMPLE SEARCH INITIATED 15:37:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 13676 TO ITERATE
```

7.3% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
PROJECTED ITERATIONS: 266519 TO 280521
PROJECTED ANSWERS: 0 TO 0
BATCH **COMPLETE**

L2 0 SEA SSS SAM L1

=> s 11 full
FULL SEARCH INITIATED 15:37:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 275040 TO ITERATE

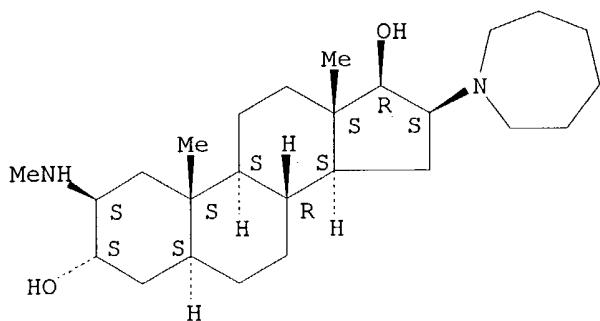
100.0% PROCESSED 275040 ITERATIONS 122 ANSWERS
SEARCH TIME: 00.00.11

L3 122 SEA SSS FUL L1

=> d scan

L3 122 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Androstane-3,17-diol, 16-(hexahydro-1H-azepin-1-yl)-2-(methylamino)-,
(2 β ,3 α ,5 α ,16 β ,17 β)- (9CI)
MF C26 H46 N2 O2

Absolute stereochemistry.

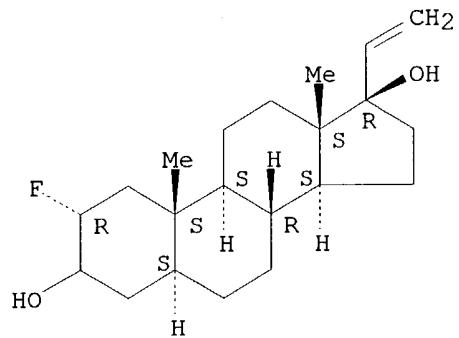


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L3 122 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 5 α ,17 α -Pregn-20-ene-3,17-diol, 2 α -fluoro- (7CI)
MF C21 H33 F 02

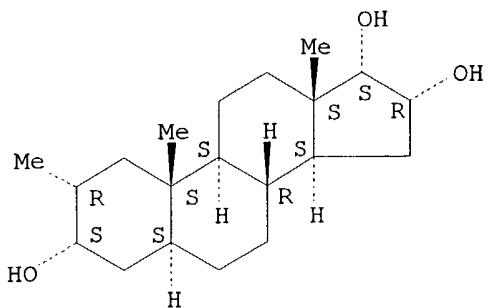
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 122 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Androstane-3,16,17-triol, 2-methyl-, (2 α ,3 α ,5 α ,16 α ,17 α)- (9CI)
MF C20 H34 O3

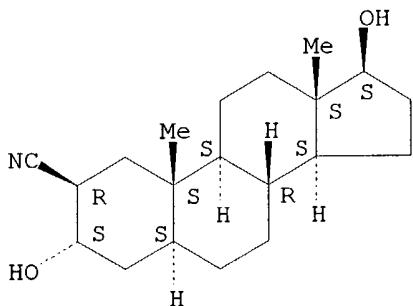
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 122 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
 IN 5 α -Androstan-2 β -carbonitrile, 3 α ,17 β -dihydroxy-
 (7CI, 8CI)
 MF C20 H31 N O2

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	155.42	155.63

FILE 'CAPLUS' ENTERED AT 15:38:14 ON 15 MAR 2004
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 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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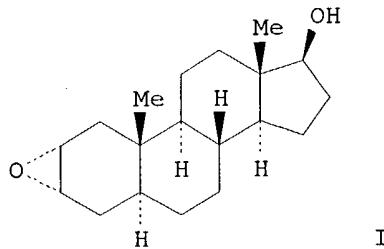
FILE COVERS 1907 - 15 Mar 2004 VOL 140 ISS 12
FILE LAST UPDATED: 14 Mar 2004 (20040314/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L4 75 L3

=> d 1-10 ibib abs hitstr

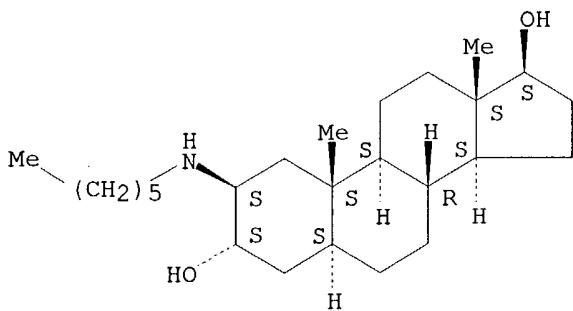
L4 ANSWER 1 OF 75 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:513220 CAPLUS
DOCUMENT NUMBER: 139:323692
TITLE: An efficient method for the regioselective aminolysis of 2,3 α -steroidal epoxide
AUTHOR(S): Thibeault, Dominic; Poirier, Donald
CORPORATE SOURCE: Medicinal Chemistry Division, Oncology and Molecular Endocrinology Research Centre, Centre Hospitalier Universitaire de Quebec (CHUQ) and Universite Laval, Sainte-Foy, QC, G1V 4G2, Can.
SOURCE: Synlett (2003), (8), 1192-1194
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:323692
GI



I

AB The opening of hindered 2,3 α -steroidal epoxide I with primary and secondary amines was performed nearly quant. with a catalytic amount of Gd(OTf)₃ in toluene in a sealed tube at high temperature. This new method is much more efficient (48-97% yields) than the older classical one (0-64% yields) using a large excess of amine.
IT 613661-87-3P 613661-88-4P 613661-89-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(efficient method for regioselective aminolysis of 2,3 α -steroidal epoxide)
RN 613661-87-3 CAPLUS
CN Androstane-3,17-diol, 2-(hexylamino)-, (2 β ,3 α ,5 α ,17 β)- (9CI) (CA INDEX NAME)

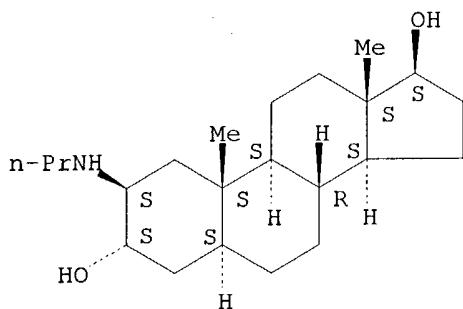
Absolute stereochemistry.



RN 613661-88-4 CAPLUS

CN Androstane-3,17-diol, 2-(propylamino)-, (2β,3α,5α,17.β)- (9CI) (CA INDEX NAME)

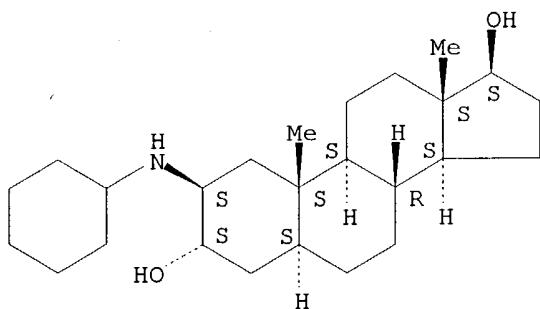
Absolute stereochemistry.



RN 613661-89-5 CAPLUS

CN Androstane-3,17-diol, 2-(cyclohexylamino)-, (2β,3α,5α,17.β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

39

THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 75 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:128467 CAPLUS

DOCUMENT NUMBER: 136:274459

TITLE: Gas chromatographic and mass spectrometric analysis of conjugated steroids in urine

AUTHOR(S): Yoon, Jong Man; Lee, Kyung Ho

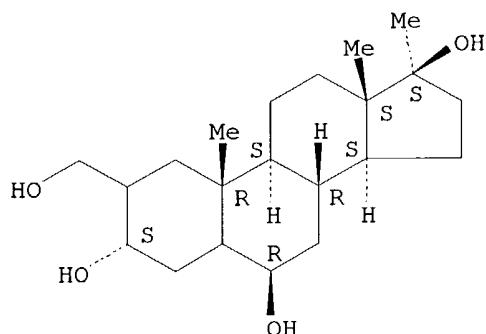
CORPORATE SOURCE: Department of Marine Biomedical Science, College of Ocean Science and Technology, Kunsan National

SOURCE: University, Jeollabuk-do, 573-702, S. Korea
Journal of Biosciences (Bangalore, India) (2001),
26(5), 627-634
CODEN: JOBSDN; ISSN: 0250-5991
PUBLISHER: Indian Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This study was carried out qual. and quant. to investigate the presence and the concns. of anabolic steroids in urine collected from orally administered humans. Microanal. of conjugated steroids by gas chromatog. and mass spectrometry (GC/MS) has been carried out. Following oral administration three major metabolites of anabolic steroid drugs have been detected and partially characterized. The six steroids can be analyzed at the same time in 17 min. The lower detection limit was 10 ng/mL in 5 mL of urine. The conjugated steroids from urine were centrifuged to 2,430 g for 10 min, the supernatant solution passed through Amberlite XAD-2 column and the steroids eluted fraction esterified by using MSTFA and TMSI. The rate of metabolism and urinary excretion seem to be reasonably fast.

IT 104413-39-0
RL: ANT (Analyte); ANST (Analytical study)
(gas chromatog. and mass spectrometric anal. of conjugated steroids in urine)
RN 104413-39-0 CAPLUS
CN Androstane-3,6,17-triol, 2-(hydroxymethyl)-17-methyl-,
(3 α ,6 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 75 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:225247 CAPLUS
DOCUMENT NUMBER: 129:660
TITLE: Gas chromatographic/mass spectrometric characterization of dromostanolone metabolites in human urine
AUTHOR(S): Kim, Taewook; Choi, Man Ho; Jung, Byung Hwa; Chung, Bong Chul
CORPORATE SOURCE: Bioanalysis and Biotransformation Research Center, Korea Institute of Science and Technology, Seoul, 136-791, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (1998), 19(2), 194-196
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The metabolism of dromostanolone (2α -methyl- 5α -androstan- 17β -ol-3-one) was studied in three adult volunteers after oral dose of 20 mg. Solvent exts. of urine obtained after enzyme hydrolysis were derivatized with MSTFA/TMCS and MSTFA/TMIS. The structures of intact drug and its metabolites were determined by gas chromatog./mass spectrometry (GC/MS) in electron impact (EI) mode. The major metabolite (2α -methyl- 5α -androstan- 3α -ol-17-one), its 3β -epimer, parent compound, and several hydroxylated metabolites including intact drug were detected by comparing total ion chromatograms of control urine with that of the administered sample. Two epimers of 2α -methyl- 5α -androstan-3,17 β -diol were detected using selected ion monitoring. The maximum excretion of dromostanolone and 2α -methyl- 5α -androstan- 3α -ol-17-one was reached in 6.2-15 h. The half-life of intact dromostanolone was 5.3 h. About 3.0% of the administered amount was found to be excreted within 95 h as unchanged form.

IT 5197-60-4 6022-07-7

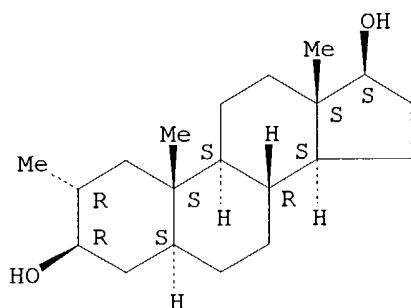
RL: ANT (Analyte); BSU (Biological study, unclassified); MFM (Metabolic formation); ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative)

(gas chromatog./mass spectrometric characterization of dromostanolone metabolites in human urine)

RN 5197-60-4 CAPLUS

CN Androstane-3,17-diol, 2-methyl-, ($2\alpha, 3\beta, 5\alpha, 17\beta$)-
(9CI) (CA INDEX NAME)

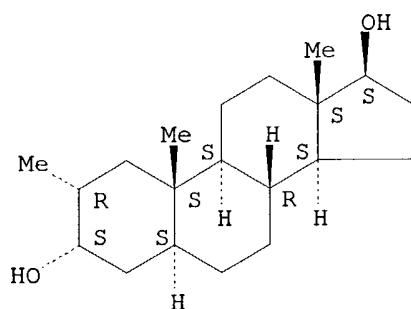
Absolute stereochemistry.



RN 6022-07-7 CAPLUS

CN Androstane-3,17-diol, 2-methyl-, ($2\alpha, 3\alpha, 5\alpha, 17\beta$)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



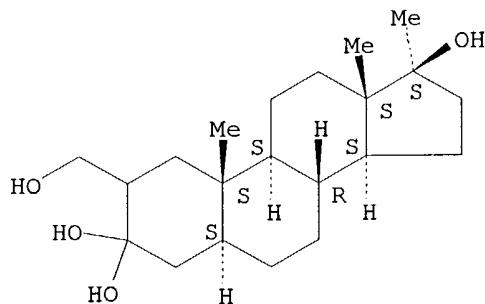
REFERENCE COUNT:

11

THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

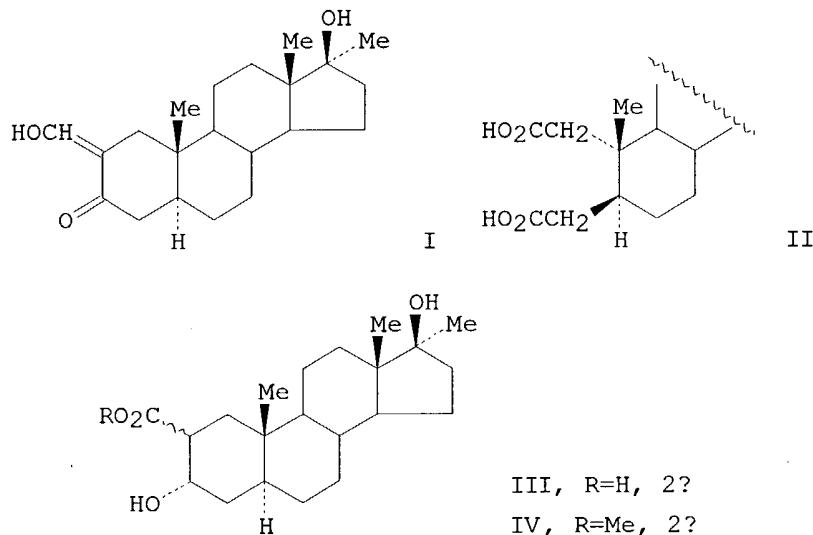
L4 ANSWER 4 OF 75 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1993:441224 CAPLUS
 DOCUMENT NUMBER: 119:41224
 TITLE: Metabolism of anabolic steroids in man: synthesis and use of reference substances for identification of anabolic steroid metabolites
 AUTHOR(S): Schaenzer, Willi; Donike, Manfred
 CORPORATE SOURCE: Dtsch. Sporthochschule Koeln, Inst. Biochem., Carl-Diem-Weg 6, 5000, Cologne, Germany
 SOURCE: Analytica Chimica Acta (1993), 275(1-2), 23-48
 CODEN: ACACAM; ISSN: 0003-2670
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The use of anabolic steroids was banned by the International Olympic Committee for the first time at the Olympic Games in Montreal in 1976. Since that time the misuse of anabolic steroids by athletes has been controlled by anal. of urine exts. by gas chromatog.-mass spectrometry (GC-MS). The excreted steroids or their metabolites, or both, are isolated from urine by XAD-2 adsorption, enzymic hydrolysis of conjugated excreted metabolites with β -glucuronidase from *Escherichia coli*, liquid-liquid extraction with di-Et ether, and converted into trimethylsilyl (TMS) derivs. The confirmation of an anabolic steroid misuse is based on comparison of the electron impact ionization (EI) mass spectrum and GC retention time of the isolated steroid and/or its metabolite with the EI mass spectrum and GC retention time of authentic reference substances. For this purpose excretion studies with the most common anabolic steroids were performed and the main excreted metabolites were synthesized for bolasterone, boldenone, 4-chlorodehydromethyltestosterone, clostebol, drostanolone, fluoxymesterone, formebolone, mestanolone, mesterolone, metandienone, methandriol, metenolone, methyltestosterone, nandrolone, norethandrolone, oxandrolone, and stanozolol. The metabolism of anabolic steroids, the synthesis of their main metabolites, their GC retention and EI mass spectra as TMS derivs. are discussed.
 IT 148505-58-2
 RL: BIOL (Biological study)
 (as oxymetholone metabolite, in urine of human)
 RN 148505-58-2 CAPLUS
 CN Androstane-3,3,17-triol, 2-(hydroxymethyl)-17-methyl-, (5 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 5 OF 75 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1993:52632 CAPLUS
 DOCUMENT NUMBER: 118:52632
 TITLE: Studies on anabolic steroids. 10. Synthesis and identification of acidic urinary metabolites of

AUTHOR(S): oxymetholone in a human
Bi, Honggang; Masse, Robert; Just, George
CORPORATE SOURCE: Inst. Nat. Rech. Sci., Univ. Quebec, Pointe-Claire,
QC, H9R 1G6, Can.
SOURCE: Steroids (1992), 57(9), 453-9
DOCUMENT TYPE: CODEN: STEDAM; ISSN: 0039-128X
LANGUAGE: English
GI

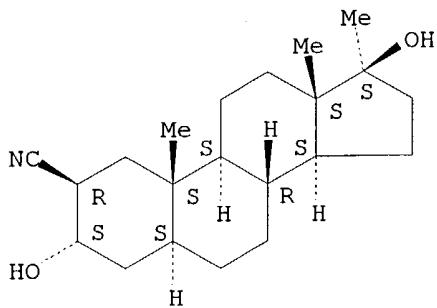


AB Two major unconjugated acidic metabolites of oxymetholone (I), e.g., 17 β -hydroxy-17 α -methyl-2,3-seco-5 α -androstane-2,3-dioic acid (II) and 3 α ,17 β -dihydroxy-17 α -methyl-5 α -androstane-2 β -carboxylic acid (III), were detected by gas chromatog./mass spectrometry in urine samples collected after oral administration of I to a human volunteer. The reference steroid II was synthesized and identified. The identification of urinary metabolite III was based on the synthesis of its stereoisomers and the isomerization of the Me ester of III to its 2-epimer, 3 α ,17 β -dihydroxy-17 α -methyl-5 α -androstane-2 α -carboxylic acid Me ester (IV). The mechanisms accounting for the formation of these acidic metabolites are discussed.

IT **141691-37-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and hydrolysis-isomerization of)

(preparation and hydrolysis isomerization of)
RN 141691-37-4 CAPLUS
CN Androstan-2-carbonitrile, 3,17-dihydroxy-17-methyl-,
(2B,3a,5a,17B)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



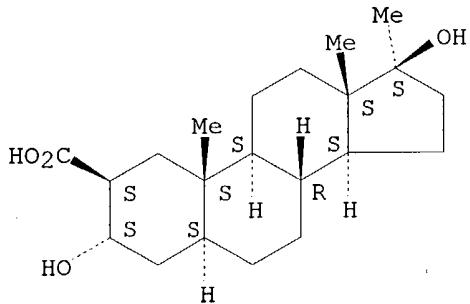
IT 141691-33-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and identification of, as oxymetholone metabolite in humans)

RN 141691-33-0 CAPLUS

CN Androstane-2-carboxylic acid, 3,17-dihydroxy-17-methyl-,
(2 β ,3 α ,5 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



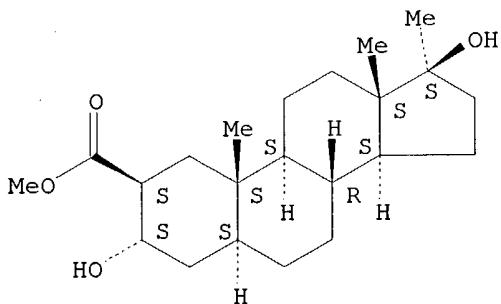
IT 145486-81-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and isomerization of)

RN 145486-81-3 CAPLUS

CN Androstane-2-carboxylic acid, 3,17-dihydroxy-17-methyl-, methyl ester,
(2 β ,3 α ,5 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



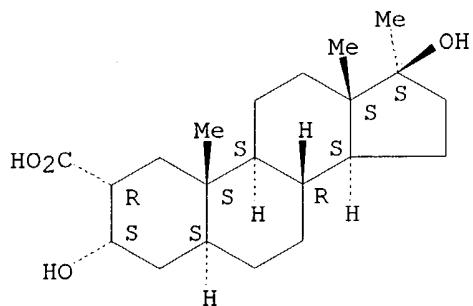
IT 141691-38-5P 145459-03-6P 145459-06-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and methylation of)

RN 141691-38-5 CAPLUS

CN Androstane-2-carboxylic acid, 3,17-dihydroxy-17-methyl-,
(2 α ,3 α ,5 α ,17 β)- (9CI) (CA INDEX NAME)

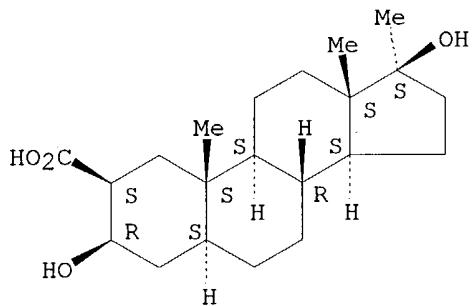
Absolute stereochemistry.



RN 145459-03-6 CAPLUS

CN Androstane-2-carboxylic acid, 3,17-dihydroxy-17-methyl-,
(2 β ,3 β ,5 α ,17 β)- (9CI) (CA INDEX NAME)

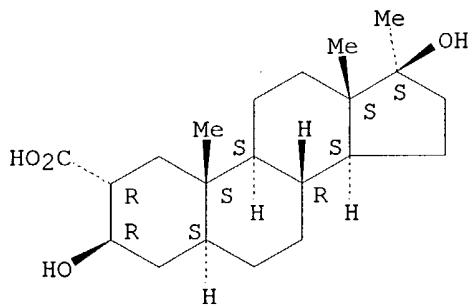
Absolute stereochemistry.



RN 145459-06-9 CAPLUS

CN Androstane-2-carboxylic acid, 3,17-dihydroxy-17-methyl-,
(2 α ,3 β ,5 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 141691-39-6P 145459-04-7P 145459-05-8P

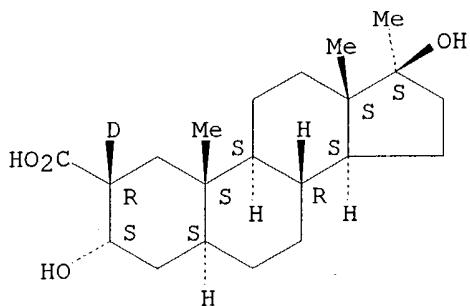
145459-07-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 141691-39-6 CAPLUS

CN Androstane-2-d-2-carboxylic acid, 3,17-dihydroxy-17-methyl-,
(2 α ,3 α ,5 α ,17 β)- (9CI) (CA INDEX NAME)

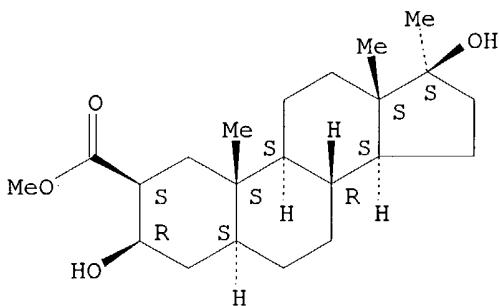
Absolute stereochemistry.



RN 145459-04-7 CAPLUS

CN Androstane-2-carboxylic acid, 3,17-dihydroxy-17-methyl-, methyl ester,
(2 β ,3 β ,5 α ,17 β)- (9CI) (CA INDEX NAME)

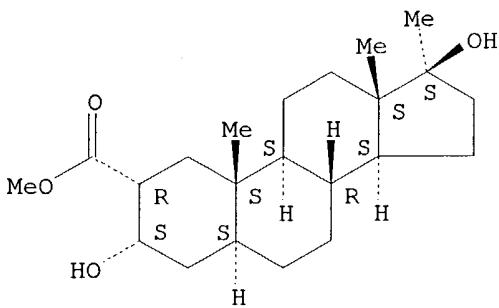
Absolute stereochemistry.



RN 145459-05-8 CAPLUS

CN Androstane-2-carboxylic acid, 3,17-dihydroxy-17-methyl-, methyl ester,
(2 α ,3 α ,5 α ,17 β)- (9CI) (CA INDEX NAME)

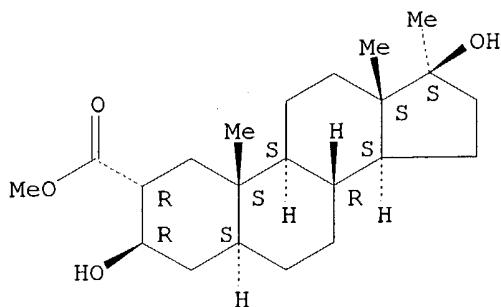
Absolute stereochemistry.



RN 145459-07-0 CAPLUS

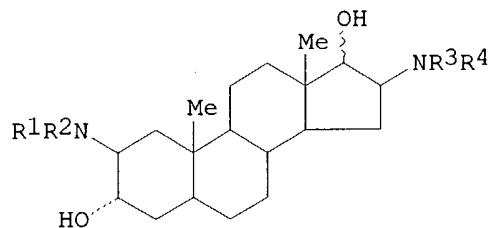
CN Androstane-2-carboxylic acid, 3,17-dihydroxy-17-methyl-, methyl ester,
(2 α ,3 β ,5 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 6 OF 75 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1992:605210 CAPLUS
 DOCUMENT NUMBER: 117:205210
 TITLE: Use of 2 β ,16 β -diamino-3 α ,17-dihydroxyandrostane derivatives for the treatment of arrhythmic disorders
 INVENTOR(S): Kellock, John; Taylor, Robert; Campbell, John; Winslow, Eileen
 PATENT ASSIGNEE(S): AKZO N. V., Neth.
 SOURCE: Eur. Pat. Appl., 11 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 496134	A1	19920729	EP 1991-203327	19911217
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
ZA 9109813	A	19921230	ZA 1991-9813	19911212
AU 9189737	A1	19920625	AU 1991-89737	19911216
AU 645869	B2	19940127		
CA 2058100	AA	19920622	CA 1991-2058100	19911219
JP 04295493	A2	19921020	JP 1991-337484	19911220
PRIORITY APPLN. INFO.:			EP 1990-314178	19901221
OTHER SOURCE(S):		MARPAT 117:205210		
GI				



I

AB The title compds. I [R1-R4 = H, C1-6 alkyl, C7-12 aralkyl, C2-6 acyl, (C1-6 alkyl-substituted) C3-7 cycloalkyl, or R1NR2 and/or R3NR4 forms a (C1-6 alkyl-substituted) 5-, 6-, or 7-membered ring; twirched line = α or β bond] and pharmaceutically acceptable salts thereof are useful for the treatment of arrhythmic disorders. The in vivo ED50 value for 22 I was determined for monophasic ventricular ECG prolongation during pacing. Tablet and injection formulations are disclosed. A tablet composition

contained 2 β ,3 α ,5 α ,16 β ,17 β -2-amino-16-(1-piperidinyl)-androstane-3,17-diol-HCl (1:2) 250, hydroxypropyl cellulose 21.0, corn starch 70.0, Mg stearate 5.25, colloidal SiO₂ 10.5 and lactose 200M to 700 mg/tablet.

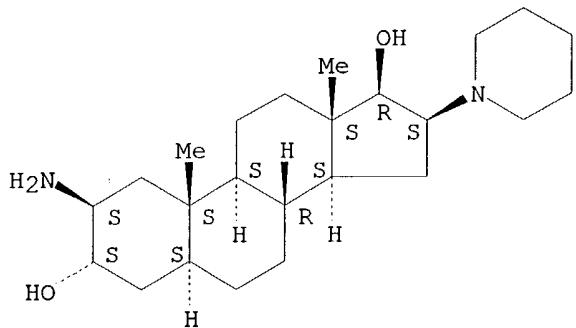
IT 128609-30-3 144209-30-3 144209-31-4
144209-32-5 144209-35-8 144209-37-0
144209-39-2 144209-40-5 144209-41-6
144209-42-7 144209-44-9 144209-46-1

RL: BIOL (Biological study)
(antiarrhythmic)

RN 128609-30-3 CAPLUS

CN Androstane-3,17-diol, 2-amino-16-(1-piperidinyl)-,
(2 β ,3 α ,5 α ,16 β ,17 β)- (9CI) (CA INDEX NAME)

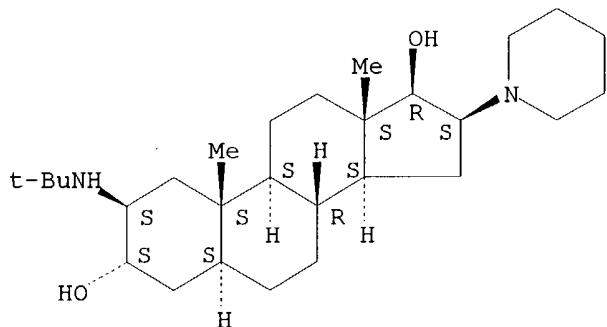
Absolute stereochemistry.



RN 144209-30-3 CAPLUS

CN Androstane-3,17-diol, 2-[(1,1-dimethylethyl)amino]-16-(1-piperidinyl)-, (2 β , 3 α , 5 α , 16 β , 17 β)- (9CI) (CA INDEX NAME)

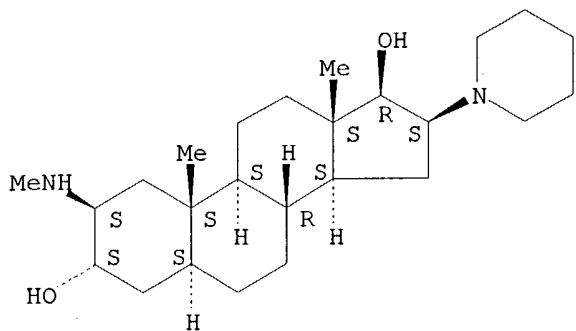
Absolute stereochemistry.



RN 144209-31-4 CAPLUS

CN Androstan-3,17-diol, 2-(methylamino)-16-(1-piperidinyl)-,
(2 β ,3 α ,5 α ,16 β ,17 β)- (9CI) (CA INDEX NAME)

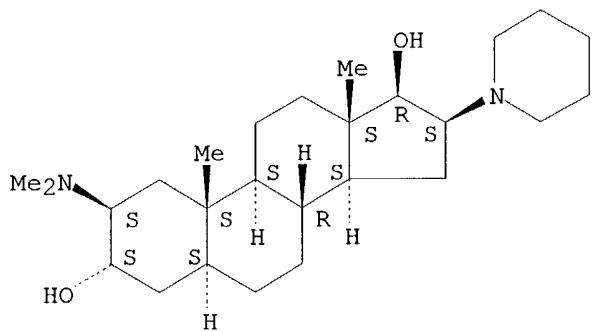
Absolute stereochemistry.



RN 144209-32-5 CAPLUS

CN Androstane-3,17-diol, 2-(dimethylamino)-16-(1-piperidinyl)-,
(2β,3α,5α,16β,17β)- (9CI) (CA INDEX NAME)

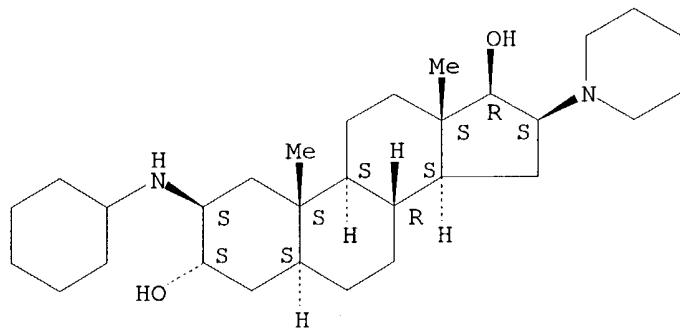
Absolute stereochemistry.



RN 144209-35-8 CAPLUS

CN Androstane-3,17-diol, 2-(cyclohexylamino)-16-(1-piperidinyl)-,
(2β,3α,5α,16β,17β)- (9CI) (CA INDEX NAME)

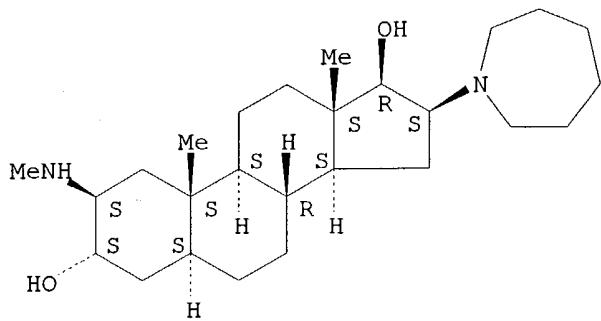
Absolute stereochemistry.



RN 144209-37-0 CAPLUS

CN Androstane-3,17-diol, 16-(hexahydro-1H-azepin-1-yl)-2-(methylamino)-,
(2β,3α,5α,16β,17β)- (9CI) (CA INDEX NAME)

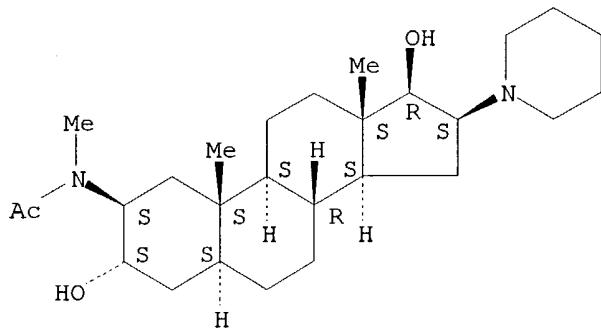
Absolute stereochemistry.



RN 144209-39-2 CAPLUS

CN Acetamide, N-[(2 β ,3 α ,5 α ,16 β ,17 β)-3,17-dihydroxy-16-(1-piperidinyl)androstan-2-yl]-N-methyl- (9CI) (CA INDEX NAME)

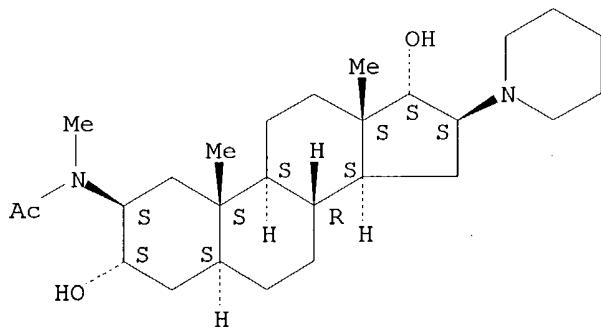
Absolute stereochemistry.



RN 144209-40-5 CAPLUS

CN Acetamide, N-[(2 β ,3 α ,5 α ,16 β ,17 α)-3,17-dihydroxy-16-(1-piperidinyl)androstan-2-yl]-N-methyl- (9CI) (CA INDEX NAME)

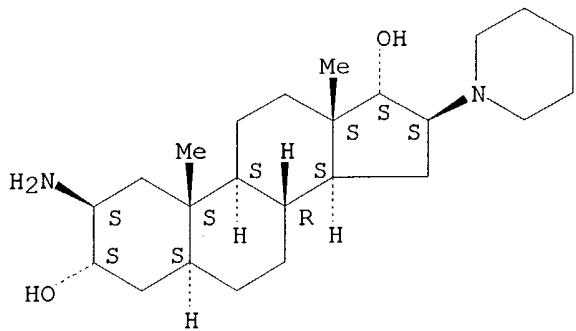
Absolute stereochemistry.



RN 144209-41-6 CAPLUS

CN Androstane-3,17-diol, 2-amino-16-(1-piperidinyl)-, (2 β ,3 α ,5 α ,16 β ,17 α)- (9CI) (CA INDEX NAME)

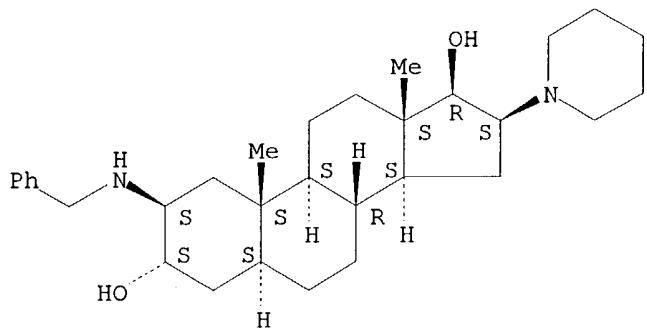
Absolute stereochemistry.



RN 144209-42-7 CAPLUS

CN Androstane-3,17-diol, 2-[(phenylmethyl)amino]-16-(1-piperidinyl)-, (2β,3α,5α,16β,17β)- (9CI) (CA INDEX NAME)

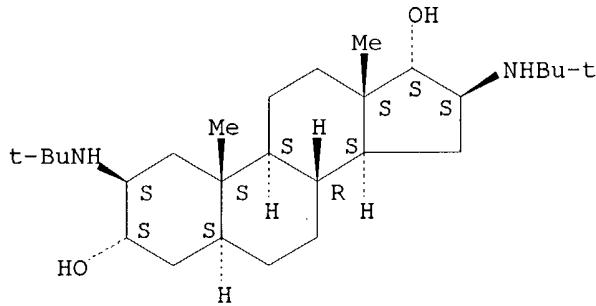
Absolute stereochemistry.



RN 144209-44-9 CAPLUS

CN Androstane-3,17-diol, 2,16-bis[(1,1-dimethylethyl)amino]-, (2β,3α,5α,16β,17α)- (9CI) (CA INDEX NAME)

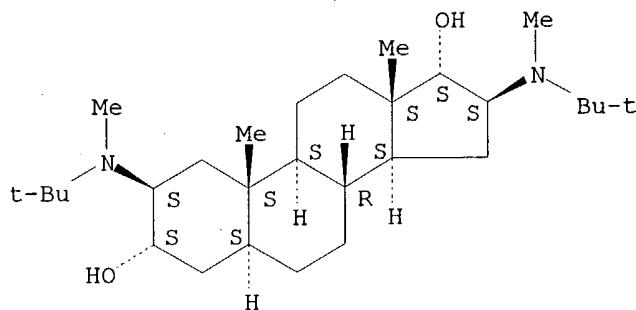
Absolute stereochemistry.



RN 144209-46-1 CAPLUS

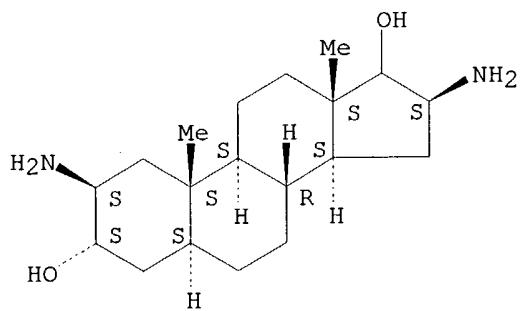
CN Androstane-3,17-diol, 2,16-bis[(1,1-dimethylethyl)methylamino]-, (2β,3α,5α,16β,17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



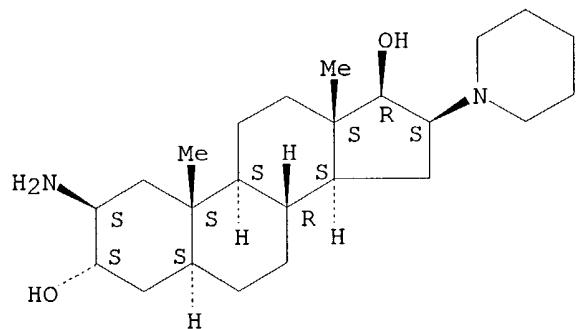
IT 144231-01-6D, derivs.
 RL: BIOL (Biological study)
 (antiarrhythmics)
 RN 144231-01-6 CAPLUS
 CN Androstane-3,17-diol, 2,16-diamino-, (2 β ,3 α ,5 α ,16 β)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 144209-47-2 144209-48-3 144209-49-4
 RL: BIOL (Biological study)
 (tablet of, for antiarrhythmic)
 RN 144209-47-2 CAPLUS
 CN Androstane-3,17-diol, 2-amino-16-(1-piperidinyl)-, dihydrochloride,
 (2 β ,3 α ,5 α ,16 β ,17 β)- (9CI) (CA INDEX NAME)

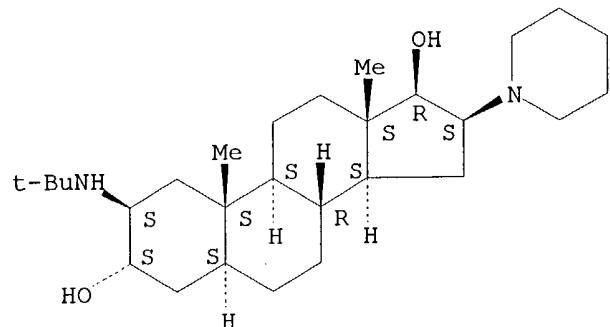
Absolute stereochemistry.



RN 144209-48-3 CAPLUS

CN Androstane-3,17-diol, 2-[(1,1-dimethylethyl)amino]-16-(1-piperidinyl)-, dihydrochloride, (2 β ,3 α ,5 α ,16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

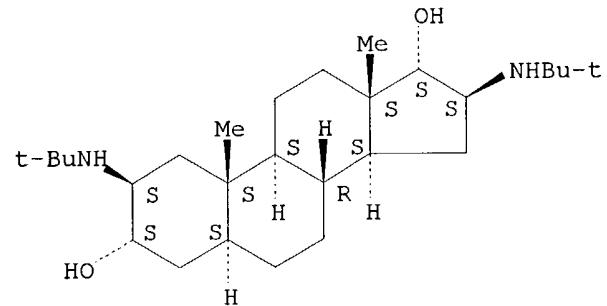


● 2 HCl

RN 144209-49-4 CAPLUS

CN Androstane-3,17-diol, 2,16-bis[(1,1-dimethylethyl)amino]-, dihydrochloride, (2 β ,3 α ,5 α ,16 β ,17 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● 2 HCl

L4 ANSWER 7 OF 75 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:463110 CAPLUS

DOCUMENT NUMBER: 117:63110

TITLE: The methyl-5 α -dihydrotestosterones mesterolone and drostanolone; gas chromatographic/mass spectrometric characterization of the urinary metabolites

AUTHOR(S): De Boer, D.; De Jong, E. G.; Maes, R. A. A.; Van Rossum, J. M.

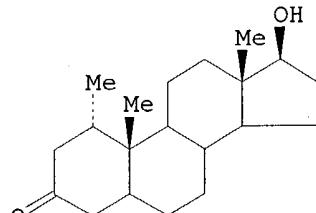
CORPORATE SOURCE: Netherlands Inst. Drugs Doping Res., Utrecht, 3584 CA, Neth.

SOURCE: Journal of Steroid Biochemistry and Molecular Biology

(1992), 42(3-4), 411-19
CODEN: JSBEBZ; ISSN: 0960-0760

DOCUMENT TYPE:
LANGUAGE:
GI

Journal
English



I

AB Before including the detection of the methyl-5α-dihydrotestosterones mesterolone (I) and its 2-Me analog drostanolone, in doping control procedures, their urinary metabolites in humans were characterized by gas chromatog./mass spectrometry. Several metabolites were found after enzymic hydrolysis and conversion of the resp. metabolites to their trimethylsilyl-enol-trimethylsilyl ether derivs. The major metabolites of I and drostanolone were identified as 1α-methyl-androsterone and 2α-methyl-androsterone, resp. The parent compds. and the intermediate 3α,17β-dihydroxy steroid metabolites were detected as well. The reduction into the corresponding 3β-hydroxy steroids was a minor metabolic pathway. All metabolites were conjugated to glucuronic acid.

IT 5197-60-4 6022-07-7

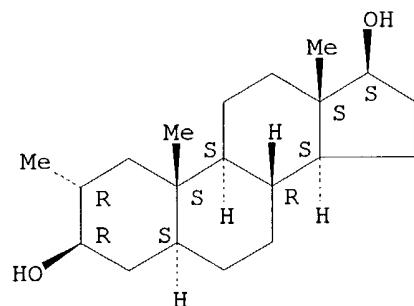
RL: PRP (Properties)

(gas chromatog.-mass spectrum of)

RN 5197-60-4 CAPLUS

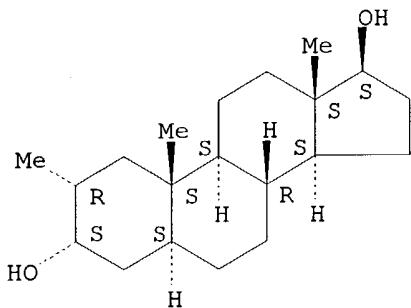
CN Androstane-3,17-diol, 2-methyl-, (2α,3β,5α,17β)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

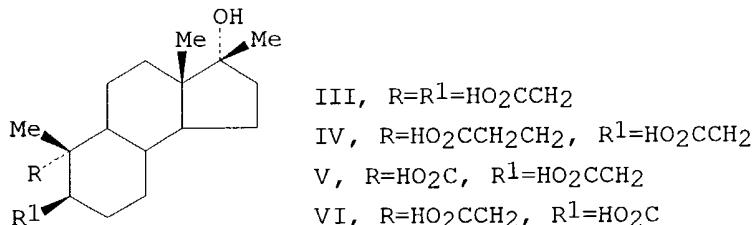
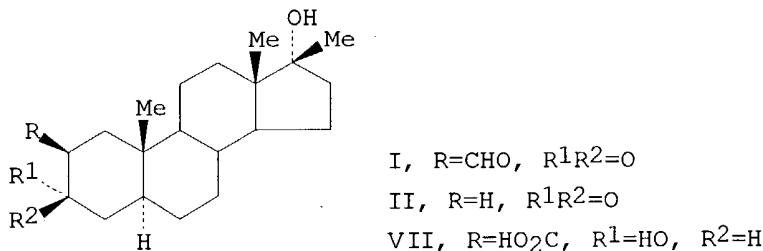


RN 6022-07-7 CAPLUS
CN Androstane-3,17-diol, 2-methyl-, (2α,3α,5α,17β)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 8 OF 75 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1992:420715 CAPLUS
 DOCUMENT NUMBER: 117:20715
 TITLE: Studies on anabolic steroids-8. GC/MS characterization of unusual seco acidic metabolites of oxymetholone in human urine
 AUTHOR(S): Bi, Honggang; Du, Ping; Masse, Robert
 CORPORATE SOURCE: Univ. Quebec, Pointe-Claire, QC, H9R 1G6, Can.
 SOURCE: Journal of Steroid Biochemistry and Molecular Biology (1992), 42(2), 229-42
 CODEN: JSBBEZ; ISSN: 0960-0760
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB One of the biotransformation routes of oxymetholone (I) in man leads to the formation of mestanolone (II). To demonstrate that this steroid may be formed by decarboxylation of an intermediate metabolite of I bearing a 2-carboxylic group, the authors studied the urinary excretion of I acidic metabolites. Five new acidic metabolites are reported here for the 1st time, among which 4 are unusual seco steroids resulting from the oxidative cleavage of the A-ring. The most abundant compound is III, the cumulative excretion of which accounted for 1.52% of the dose. Three other seco diacids were produced in smaller amounts, namely IV-VI. The fifth acidic metabolite was identified as VII. The excretion in urine of these acidic metabolites suggests that the 2-hydroxymethylene group in I is readily

oxidized to yield the corresponding β -keto acid which can be (1) decarboxylated to form mestanolone; (2) reduced at C-3 to give VII; and (3) further oxidized to afford the unexpected seco diacids III-VI. The identity of compds. III and VII was ascertained by GC/MS and ^1H and ^{13}C -NMR anal. of reference compds. The other metabolites were characterized by GC/MS anal.

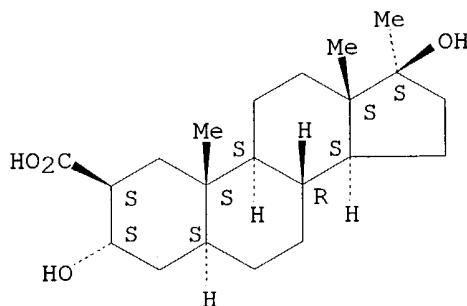
IT **141691-33-0**

RL: BIOL (Biological study)
(as oxymetholone metabolite, in human urine, gas chromatog.-mass spectra anal. of)

RN 141691-33-0 CAPLUS

CN Androstane-2-carboxylic acid, 3,17-dihydroxy-17-methyl-,
(2 β ,3 α ,5 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



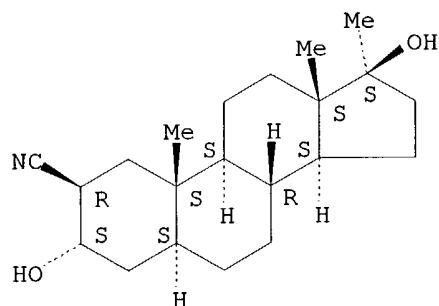
IT **141691-37-4P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 141691-37-4 CAPLUS

CN Androstane-2-carbonitrile, 3,17-dihydroxy-17-methyl-,
(2 β ,3 α ,5 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



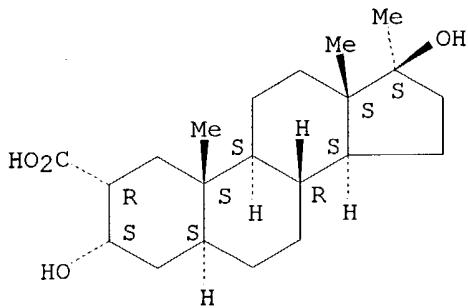
IT **141691-38-5P 141691-39-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 141691-38-5 CAPLUS

CN Androstane-2-carboxylic acid, 3,17-dihydroxy-17-methyl-,
(2 α ,3 α ,5 α ,17 β)- (9CI) (CA INDEX NAME)

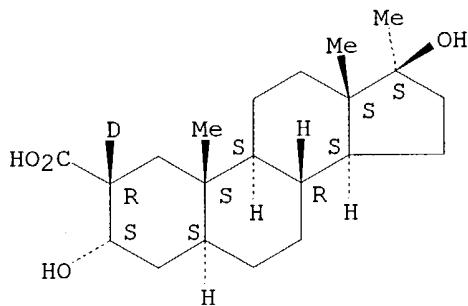
Absolute stereochemistry.



RN 141691-39-6 CAPLUS

CN Androstane-2-d-2-carboxylic acid, 3,17-dihydroxy-17-methyl-,
(2 α ,3 α ,5 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 9 OF 75 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:478806 CAPLUS

DOCUMENT NUMBER: 113:78806

TITLE: Synthesis of 3 α -amino-2 β -dihydroxy-16 β -piperidino-5 α -androstane and 2 β -amino-3 α ,17 β -dihydroxy-16 β -piperidino-5 α -androstane

AUTHOR(S): Xu, Xiaoyan; Liao, Qingjiang; Xiang, Manwen

CORPORATE SOURCE: Coll. Pharm., China Pharm. Univ., Nanjing, Peop. Rep. China

SOURCE: Youji Huaxue (1989), 9(5), 451-4

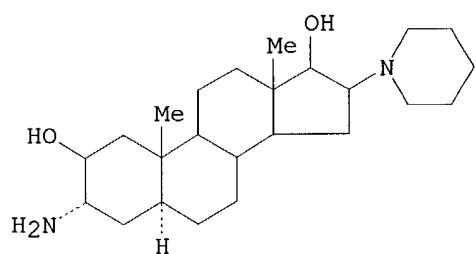
CODEN: YCHHDX; ISSN: 0253-2786

DOCUMENT TYPE: Journal

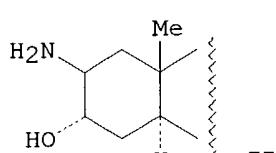
LANGUAGE: Chinese

OTHER SOURCE(S): CASREACT 113:78806

GI



I



II

AB Starting from epiandrosterone, 3α -amino- $2\beta,17\beta$ -dihydroxy- 16β -piperidino- 5α -androstan-17-one was prepared via $2\beta,3\beta$ -epoxy- 5α -androst-17-one and 2β -amino- $3\alpha,17\beta$ -dihydroxy- 16β -piperidino- 5α -androstan-17-one. An improved synthesis of 3α -azido- 2β -hydroxy- 5α -androst-17-one was described.

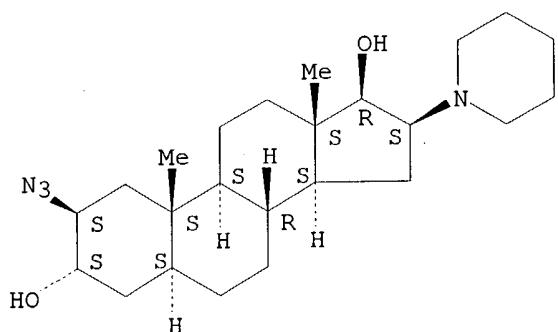
IT **128609-29-0P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 128609-29-0 CAPLUS

CN Androstane-3,17-diol, 2-azido-16-(1-piperidinyl)-, (2 β ,3 α ,5 α ,16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



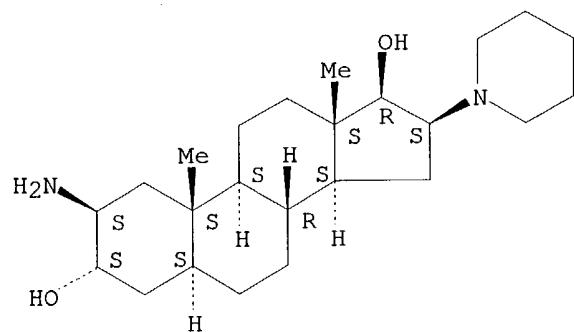
IT **128609-30-3P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 128609-30-3 CAPLUS

CN Androstane-3,17-diol, 2-amino-16-(1-piperidinyl)-, (2 β ,3 α ,5 α ,16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



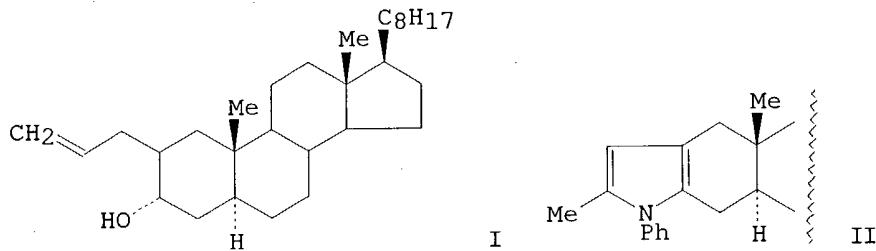
L4 ANSWER 10 OF 75 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:39241 CAPLUS

DOCUMENT NUMBER: 110:39241

TITLE: Reaction of some steroidal γ,δ -unsaturated alcohols with thallium(III) nitrate. Preparation of some steroidal derivatives having a hetero ring fused

AUTHOR(S): to the A ring
Forcellese, Maria Luigia; Cardillo, Luisa; Mincione,
Enrico
CORPORATE SOURCE: Cent. Stud. Chim. Sostanze Org. Nat., CNR, Rome,
I-00185, Italy
SOURCE: Gazzetta Chimica Italiana (1988), 118(6), 465-8
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:39241
GI



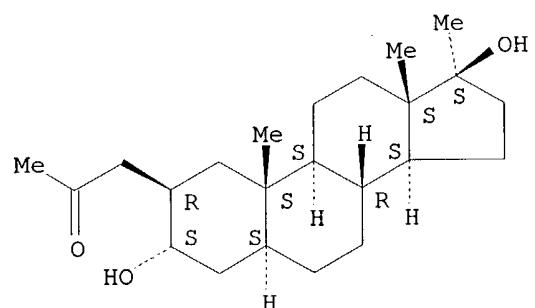
AB Tl(No₃)₃ reacts with steroid γ,δ -unsatd. alcs. to give THF derivs. and γ -hydroxy ketones. Oxidation of these latter leads to 1,4-dicarbonyl compds. that are converted into pyrrole or furan derivs. Thus, cholestanone I was converted into pyrrole II.

IT **118348-59-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and

RN 118348-59-7 CAPLUS
CN 2-Propanone, 1-[(2 β , 3 α , 5 α , 17 β)-3,17-dihydroxy-17-methylandrostan-2-yl]- (9CI) (CA INDEX NAME)

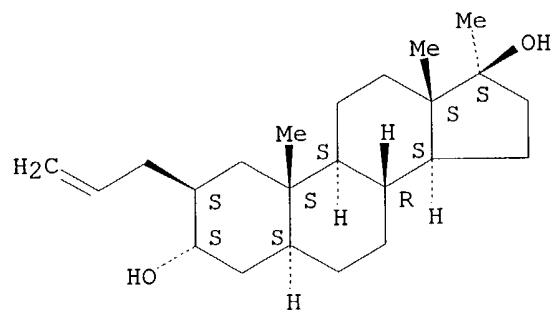
Absolute stereochemistry.



IT **57901-47-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Reaction and reaction with thallium nitrate)

RN 57901-47-0 CAPLUS
CN Androstane-3,17-diol, 17-methyl-2-(2-propenyl)-,
(2 β .3 α .5 α .17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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NEWS 10 DEC 08 CABA reloaded with left truncation
NEWS 11 DEC 08 IMS file names changed
NEWS 12 DEC 09 Experimental property data collected by CAS now available in REGISTRY
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NEWS 14 DEC 17 DGENE: Two new display fields added
NEWS 15 DEC 18 BIOTECHNO no longer updated
NEWS 16 DEC 19 CROPU no longer updated; subscriber discount no longer available
NEWS 17 DEC 22 Additional INPI reactions and pre-1907 documents added to CAS databases
NEWS 18 DEC 22 IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
NEWS 19 DEC 22 ABI-INFORM now available on STN
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NEWS 21 JAN 27 A new search aid, the Company Name Thesaurus, available in CA/CAplus
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NEWS 25 MAR 03 FRANCEPAT now available on STN

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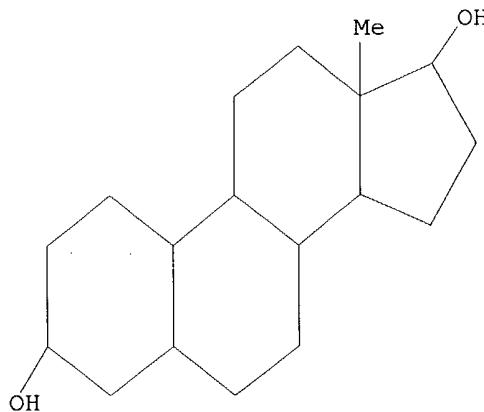
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<http://www.cas.org/ONLINE/DBSS/registryss.html>

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38 ANSWERS

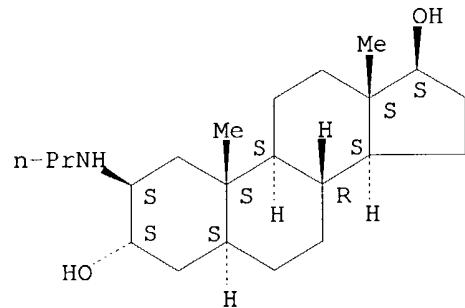
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BATCH **COMPLETE**
PROJECTED ITERATIONS: 202916 TO 215164
PROJECTED ANSWERS: 6748 TO 9138

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L2 ANSWER 1 OF 38 REGISTRY COPYRIGHT 2004 ACS on STN
RN 613661-88-4 REGISTRY
CN Androstan-3,17-diol, 2-(propylamino)-, (2 β ,3 α ,5 α ,17. β eta
.)-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
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SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



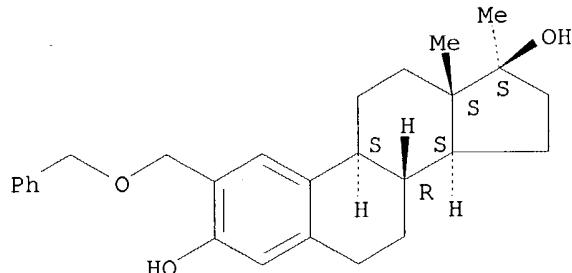
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d 12 38

L2 ANSWER 38 OF 38 REGISTRY COPYRIGHT 2004 ACS on STN
RN 15410-34-1 REGISTRY
CN Estra-1,3,5(10)-triene-3,17 β -diol, 2-[(benzyloxy)methyl]-17-methyl-
(7CI, 8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H34 O3
LC STN Files: CA, CAOLD, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d 12 35

L2 ANSWER 35 OF 38 REGISTRY COPYRIGHT 2004 ACS on STN

RN 51911-17-2 REGISTRY

CN Androstan-3,17-diol, 4-methyl-, (3 β ,4 α ,5 α ,17 β)-
(9CI) (CA INDEX NAME)

OTHER NAMES:

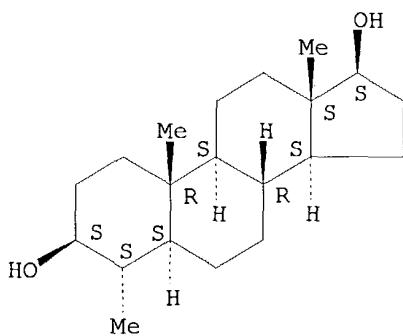
CN 4 α -Methyl-5 α -androstan-3 β -17 β -diol

FS STEREOSEARCH

MF C20 H34 O2

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=>

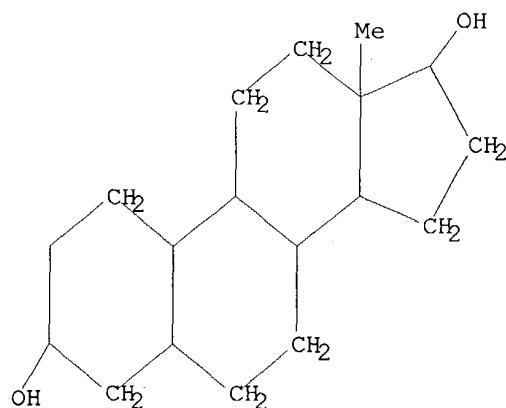
Uploading C:\STNEXP4\50.str

L3 STRUCTURE UPLOADED

=> d

L3 HAS NO ANSWERS

L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 13

SAMPLE SEARCH INITIATED 14:10:05 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 10452 TO ITERATE

9.6% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

5 ANSWERS

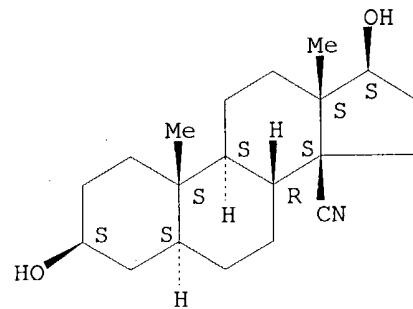
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 202916 TO 215164
PROJECTED ANSWERS: 612 TO 1478

L4 5 SEA SSS SAM L3

=> d 14 5

L4 ANSWER 5 OF 5 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21935-69-3 REGISTRY
CN 5 α ,14 β -Androstane-14-carbonitrile, 3 β ,17 β -dihydroxy-
(8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H31 N O2

Absolute stereochemistry.

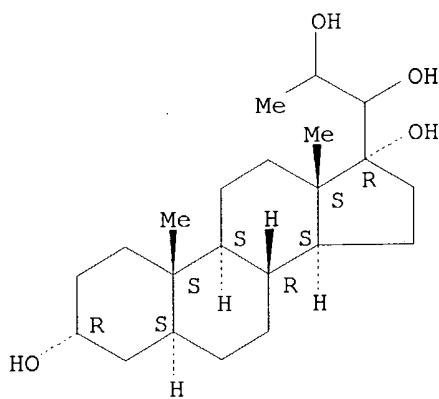


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

=> d 14 2-4

L4 ANSWER 2 OF 5 REGISTRY COPYRIGHT 2004 ACS on STN
RN 446293-54-5 REGISTRY
CN Androstane-3,17-diol, 17-(1,2-dihydroxypropyl)-,
(3 α ,5 α ,17 α)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H38 O4
SR Reaction Database
LC STN Files: CASREACT

Absolute stereochemistry.



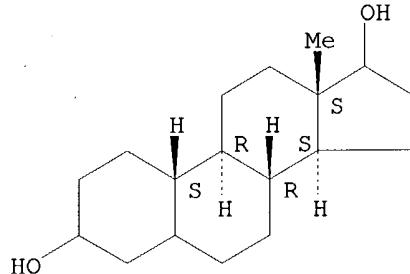
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 3 OF 5 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 123714-04-5 REGISTRY
 CN Estradiene-3,17-diol (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C18 H26 O2
 CI IDS
 SR CA
 LC STN Files: CA, CAPLUS

CM 1

CRN 65556-20-9
 CMF C18 H30 O2

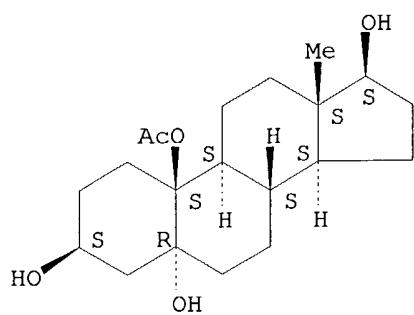
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 4 OF 5 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 56016-52-5 REGISTRY
 CN Estrane-3,5,10,17-tetrol, 10-acetate, (3β,5α,17β)- (9CI)
 (CA INDEX NAME)
 OTHER NAMES:
 CN 10-Acetoxy-5α-estrane-3β,5,17β-triol
 FS STEREOSEARCH
 MF C20 H32 O5
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)